

NLTE abundances of C, O, Ca, Ti, and Fe in the reference BAF-type stars

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Abstract. We present accurate methods of abundance determination based on the non-local thermodynamic equilibrium (NLTE) line formation for carbon, oxygen, calcium, titanium, and iron in the atmospheres of BAF-type stars. For C I-II, O I, Ca I-II, and Ti I-II, their comprehensive model atoms were described in our previous papers. A fairly complete model atom of Fe I-II is first applied in this study. We determine the NLTE abundances of the nine BAF-type stars with well-determined atmospheric parameters, using high-resolution and high signal-to-noise ratio spectral observations in the broad wavelength range, from the UV to the IR. For C, Ca, Ti, and Fe, NLTE leads to consistent abundances from the lines of the two ionisation stages. The C I, Ca II, and Fe II emission lines were detected in the near IR spectrum of the late B-type subgiant star HD 160762. They are well reproduced in the classical hydrostatic model atmosphere, when applying our NLTE methods.

Keywords. line: formation, stars: abundances, stars: atmospheres, fundamental parameters.

Chemical abundances of BAF-type unevolved stars represent abundances of the galactic matter at modern epoch. Models of stellar interior structure and evolution depend on opacity and require accurate chemical abundances. Iron is a key element for determination of stellar atmosphere parameters. To derive accurate element abundance, one needs to explore how the deviations from local thermodynamic equilibrium (LTE) affect the formation of the element lines. For the first time, we investigate the statistical equilibrium of iron in the atmospheres of BAF stars using a *comprehensive* model atom of Fe I-II. The model atom presented by Mashonkina *et al.* (2011) was upgraded by including the measured and predicted high-excitation (> 10 eV) energy levels of Fe II, as available in R. Kurucz database (<http://kurucz.harvard.edu/atoms.html>). For BAF stars, NLTE leads to weakened Fe I lines and to positive NLTE abundance corrections, in agreement with Rentzsch-Holm (1996), however, their magnitude is smaller compared to that in the earlier paper. Lines of Fe II are strengthened in NLTE, and the effect grows with line strength. The statistical equilibrium calculations for C I-II, O I, Ca I-II, and Ti I-II were performed using the methods described in Alexeeva *et al.* (2016), Sitnova *et al.* (2013), Mashonkina *et al.* (2007), and Sitnova *et al.* (2016), respectively.

We selected the nine well-studied stars, which do not reveal any pulsation activity, chemical stratification, and magnetic field. Atmospheric parameters were derived in our earlier studies by the common method based on multi-colour photometry, analysis of Balmer lines and metal lines in high-resolution spectra, and a comparison of the spectrophotometric data with the theoretical flux. They cover the following ranges in effective temperature: $7250 \text{ K} \leq T_{\text{eff}} \leq 17500 \text{ K}$, surface gravity: $3.55 \leq \log g \leq 4.30$, and metallicity: $-0.30 \leq [\text{Fe}/\text{H}] \leq 0.45$.

We determined the NLTE and LTE abundances of carbon, oxygen, calcium, titanium, and iron in the reference stars. For each species, NLTE leads to smaller line-to-line scatter compared to LTE. For the majority of stars, we obtained smaller differences in the NLTE than in the LTE abundances between the neutral and singly ionised species. For example, in LTE, the abundance discrepancy between Fe I and Fe II reaches 0.22 dex. The exception is HD 17081, where Fe I and Fe II agree in LTE, while NLTE leads to Fe I – Fe II = 0.11 dex. For the same star, we obtain C I – C II = 0.13 dex in NLTE, while –0.31 dex in LTE. An upward revision of T_{eff} , by about 80 K, can provide consistent NLTE abundances from neutrals and first ions in HD 17081.

Lines of Fe I and Fe II are widely used for atmospheric parameter determination. We evaluated how NLTE affects the results. For atmosphere with $T_{\text{eff}}/\log g/[\text{Fe}/\text{H}]/V_{\text{mic}} = 10000/4.0/0.0/2.0$, NLTE leads to an average abundance shift Fe I (NLTE) – Fe I (LTE) = 0.09 dex. To get consistent abundances from Fe I and Fe II in LTE, one needs to assume either 0.20 dex lower $\log g$ or 130 K higher T_{eff} , when the other parameter is fixed. NLTE leads to a downward revision of the microturbulent velocity because the deviations from LTE are larger for stronger lines of Fe II. For example, LTE requires an 0.2 km s^{-1} larger V_{mic} for HD 145788 (9750/3.70/0.0/1.8) than in NLTE. We found a qualitatively similar, but stronger effect on the V_{mic} determinations based on the Ti II lines (see Sitnova *et al.* 2016 for details).

In the near IR spectrum of HD 160762 (17500/3.8), the hottest star of our sample, we found emission lines of C I, Ca II, and Fe II. These lines have the same Doppler width and radial velocity as the absorption spectral lines in HD 160762. We explain these phenomena by the NLTE effects in the classical plane-parallel model atmosphere. The C I emission line formation was described in details by Alexeeva *et al.* (2016). In the atmosphere of HD 160762, Fe III is the majority species, such that $N(\text{FeIII})/N(\text{FeII}) \geq 100$. Overionisation of Fe II results in depleted energy levels and, hence, weakened Fe II lines. In case of the high-excitation lines, they either disappear or come into emission. The same happens with the Ca II high-excitation lines.

Conclusions. The NLTE calculations with a comprehensive model atom of Fe I–II were performed for the first time for the selected BAF-type stars. For the same stars, we determined the NLTE and LTE abundances of carbon, oxygen, calcium, titanium, and iron. For each element, NLTE reduces the line-to-line scatter compared to the LTE case and leads to consistent abundances from lines of the neutral and singly-ionised species. We can reproduce the emission lines of C I, Ca II, and Fe II observed in the near-IR spectrum of the late B-type star HD 160762 using our NLTE methods with the classical plane-parallel and LTE model atmosphere. For the atmospheric parameters of the A0 main-sequence star, the LTE analysis of Fe I and Fe II lines leads to an overestimation of T_{eff} , by 130 K, or an underestimation of $\log g$, by 0.20 dex.

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